WEST Search History

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DATE: Wednesday, March 02, 2005

Hide?	Set Name	Query	Hit Count
		DB=PGPB; PLUR=YES; OP=ADJ	
☐	L37	L32 and (stability)	1
☐	L36	L32 and (stable)	0
☐	L35	L32 and (stable adj2 air)	0
☐	L34	L32 and (absence adj2 solvent)	0
☐	L33	L32 and quantum yield	1
☐	L32	20030178607	1
		DB=USPT; PLUR=YES; OP=ADJ	
☐	L31	6783814.pn.	1
		DB=PGPB,USPT,USOC,EPAB,JPAB,DWPI,TDBD; PLUR=YES; OP=ADJ	
☐	L30	(persistence adj2 nm)	1
☐	L29	polymer with (persistence adj2 nm)	0
☐	L28	L26 and iptycene	6
☐	L27	L26 and fluorescen$3	10
☐	L26	L25 or l24 or l23	132
☐	L25	zhu-zhengguo$.in.	4
☐	L24	long-timothy$.in.	109
☐	L23	swager-timothy$.in.	25
		DB=USPT,EPAB,JPAB,DWPI; PLUR=YES; OP=ADJ	
☐	L22	l21 and fluorescence with yield	4
		DB=PGPB,USPT; PLUR=YES; OP=ADJ	
☐	L21	US-4356429-$.DID. OR US-4687732-$.DID. OR US-4927768-$.DID. OR US-4946890-$.DID. OR US-4992302-$.DID. OR US-5155149-$.DID. OR US-5194393-$.DID. OR US-5236808-$.DID. OR US-5244813-$.DID. OR US-5254633-$.DID. OR US-5364797-$.DID. OR US-5414069-$.DID. OR US-5451683-$.DID. OR US-0551547-$.DID. OR US-5512490-$.DID. OR US-5532129-$.DID. OR US-5540999-$.DID. OR US-5546889-$.DID. OR US-5554747-$.DID. OR US-5556524-$.DID. OR US-5563056-$.DID. OR US-5565322-$.DID. OR US-5580527-$.DID. OR US-5585646-$.DID. OR US-5591787-$.DID. OR US-5597890-$.DID. OR US-5607864-$.DID. OR US-5679773-$.DID. OR US-5700696-$.DID. OR US-5705348-$.DID. OR US-5709994-$.DID. OR US-5710197-$.DID. OR US-5723218-$.DID. OR US-5869562-$.DID. OR US-6020426-$.DID. OR US-6259277-$.DID.	36
		DB=PGPB,USPT,USOC,EPAB,JPAB,DWPI,TDBD; PLUR=YES; OP=ADJ	

☐	L20	L19 and alkoxyamine	5
☐	L19	L18 orl17 or l16	665
☐	L18	ujikawa-norihisa$.in.	5
☐	L17	nakamura-tomoyuki$.in.	192
☐	L16	hayashi-masaki$.in.	665
		DB=USPT,USOC; PLUR=YES; OP=ADJ	
☐	L15	3969071.pn.	1
		DB=PGPB,USPT,USOC,EPAB,JPAB,DWPI,TDBD; PLUR=YES; OP=ADJ	
☐	L14	(alkoxybenzene or methoxybenzene)(sulfonic) with (polymer$7 or poly or polycondensation or condensation or $3ion exchange)	5
☐	L13	alkoxybenzene sulfonic with (polymer$7 or poly or polycondensation or condensation)	0
☐	L12	L10 not l9	1
☐	L11	L10 not l8	0
☐	L10	L8 and (poly or polymer$7 or polycondensation)	12
☐	L9	L8 and (polymer$7 or polycondensation)	11
☐	L8	(sulfonated or sulfated or sulfonic) adj3 ($2methoxy benzene or $2methoxybenzene)	19
☐	L7	(sulfonated or sulfated or sulfonic) adj ($2methoxy benzene or $2methoxybenzene)	1
☐	L6	(sulfonated or sulfated or sulfonic) with methoxy benzene	181
☐	L5	l2 same (sulfonated or sulfated or sulfonic)	6
☐	L4	l2 same (sulfonated or sulfated or sulfo)	0
☐	L3	(sulfonated or sulfated or sulfo)with L2	0
☐	L2	(polymer&7 or poly$5)with (DMB or dimethoxybenzene or dialkoxybenzene or dibutoxybenzene)	181
☐	L1	(polymer&7 or poly$5)adj2 (DMB or dimethoxybenzene or dialkoxybenzene or dibbutoxybenzene)	9

END OF SEARCH HISTORY

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FILE 'REGISTRY'
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     FILE 'HCAPLUS'
L1           368 S SWAGER ?/AU
L2          2660 S ZAHN ?/AU
L3             2 S L1 AND L2
                 SEL L3 1-2 RN

     FILE 'REGISTRY'
L4             2 S E1-E2

     FILE 'LREGISTRY'
L5               STR
L6               STR

     FILE 'REGISTRY'
L7             0 S L5 AND L6
L8             0 S L5
L9               STR
L10            0 S L9
L11            2 S L9 FUL
                 SAV L11 ZEM041/A

     FILE 'CAOLD'
L12            0 S L11

     FILE 'ZCAPLUS'
L13            1 S L11

     FILE 'REGISTRY'


=> d l11 que stat
L9               STR
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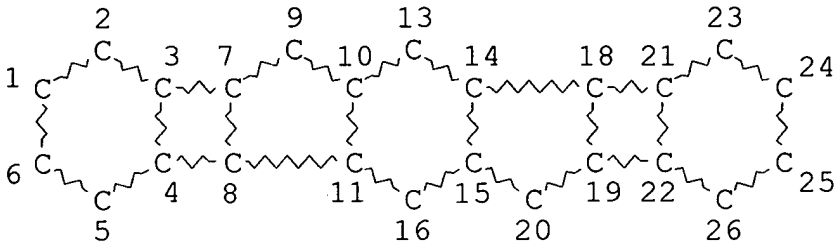

NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 24

STEREO ATTRIBUTES: NONE
L11 2 SEA FILE=REGISTRY SSS FUL L9

100.0% PROCESSED 382715 ITERATIONS 2 ANSWERS
SEARCH TIME: 00.00.07

=> file zcaplus
FILE 'ZCAPLUS'
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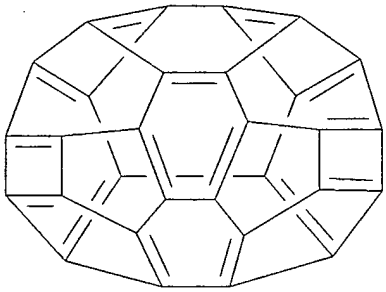
=> d l13 1 all hitstr

L13 ANSWER 1 OF 1 ZCAPLUS COPYRIGHT 2005 ACS on STN
AN 2000:619390 ZCAPLUS
DN 134:21651
ED Entered STN: 06 Sep 2000
TI Special geminals and Schlegel diagrams of molecular structures of fullerenes and metallofullerenes
AU Chiu, Y.-N.; Xiao, J.; Merritt, C. D.; Liu, K.; Huang, W.-X.; Ganelin, P. V.; Li, N. N.
CS Department of Chemistry, Center for Molecular Dynamics and Energy Transfer, The Catholic University of America, Washington, DC, 20064, USA

SO THEOCHEM (2000), 530(1,2), 67-83
CODEN: THEODJ; ISSN: 0166-1280
PB Elsevier Science B.V.
DT Journal
LA English
CC 65-3 (General Physical Chemistry)
AB Schlegel diagrams were used to demonstrate the location of geminals for the following mol. systems: C42H28 .fwdarw. C42 (C2v, D2h), C30H18 .fwdarw. C30 (C2v, D5h), C4H4 (D4h), C4H6, C28 (Td), Ti@C28 (Td), Sc3@C82 (C3v), and Sc@C20 (D5).
ST geminal Schlegel diagram fullerene metallofullerene
IT Wave function
(geminal; geminals and Schlegel diagrams of fullerenes and metallofullerenes)
IT Molecular orbital
Molecular structure-property relationship
Molecular topology
(geminals and Schlegel diagrams of fullerenes and metallofullerenes)
IT Fullerenes
Fullerides
(geminals and Schlegel diagrams of fullerenes and metallofullerenes)
IT 106-99-0, 1,3-Butadiene, properties 517-51-1 1120-53-2, 1,3-Cyclobutadiene 10075-85-1 115383-19-2, [5,6]Fullerene-C28-Td 135026-72-1, [5,6]Fullerene-C30-D5h 145077-51-6 146750-44-9 309242-94-2, [5,6,7]Fullerene-C42-C2v 309242-95-3, [4,5,6,7]Fullerene-C42-D2h 309242-96-4, [4,5,6]Fullerene-C30-C2v 309242-97-5, [4,5,6,7]Fullerene-C42-C2v **309242-98-6**, [4,5,6]Fullerene-C30-C2v 309244-06-2
(geminals and Schlegel diagrams of fullerenes and metallofullerenes)
RE.CNT 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) Baum, R; Chem Engng News 1988, V29, P33
(2) Chiu, Y; Acta Phys Hungarica 1994, V74(4), P427 ZCAPLUS
(3) Chiu, Y; Chem J Chin Univ 1997, V18, P1147 ZCAPLUS
(4) Chiu, Y; Eur J Solid State Inorg Chem 1993, Vt30, P1119
(5) Chiu, Y; J Chin Chem Soc 1992, V37, P361
(6) Chiu, Y; J Mol Struct (Theochem) 1993, V283, P13
(7) Chiu, Y; J Mol Struct (Theochem) 1994, V312, P215
(8) Chiu, Y; J Mol Struct (Theochem) 1995, V332, P47 ZCAPLUS
(9) Chiu, Y; J Mol Struct (Theochem) 1997, V389, P37 ZCAPLUS
(10) Chiu, Y; Phys Rev B 1997, V55, P6022 ZCAPLUS
(11) Cotton, F; Chemical Application of Group Theory 1990
(12) Ganelin, P; Fullerenes, Recent Advances in the Chemistry and Physics of Fullerenes and Related Materials 1994
(13) Kato, T; J Phys Chem 1997, V97, P13425

(14) Kroto, H; Nature 1987, V329, P529 ZCAPLUS
(15) Kroto, H; Nature 1995, V318, P162
(16) Manalopoulos, D; Chem Phys Lett 1991, V187, P11
(17) Merritt, C; PhD thesis, The Catholic University of America 1998
(18) Moro, L; J Phys Chem 1997, V97, P6801
(19) Reeves, M; Phys Rev B 1993, V47, P6065 ZCAPLUS
(20) Sarkas, H; J Phys Chem 1996, V100, P5169 ZCAPLUS
(21) Schmalz, T; J Am Chem Soc 1988, V110, P113
IT **309242-98-6**, [4,5,6]Fullerene-C30-C2v
(geminals and Schlegel diagrams of fullerenes and metallofullerenes)
RN 309242-98-6 ZCAPLUS
CN [4,5,6]Fullerene-C30-C2v (9CI) (CA INDEX NAME)



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STRUCTURE FILE UPDATES: 28 FEB 2005 HIGHEST RN 839671-97-5
DICTIONARY FILE UPDATES: 28 FEB 2005 HIGHEST RN 839671-97-5

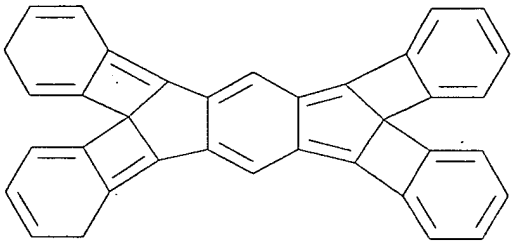
=> d l11 1 fide

L11 ANSWER 1 OF 2 REGISTRY COPYRIGHT 2005 ACS on STN
RN 334833-14-6 REGISTRY
ED Entered STN: 07 May 2001
CN 1H,6H-Tetrakisbenzo[3,4]cyclobut[1,2-a:1',2'-b:1'',2''-g:1''',2'''-h]-s-indacene (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C36 H20

CI RPS
SR CA Index Guide or Ring Systems Handbook

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C4-C4-C4-C4- C5-C5-C6-C6- C6-C6-C6	C4-C4-C4-C4- C5-C5-C6-C6- C6-C6-C6	4-4-4-4-5-5- 6-6-6-6-6	C36	86620.1.2	1



(This compound is not actually cited in any abstracts or citations. It just was registered by a company and assigned a registry number and index name by Chemical Abstracts.)

Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	503742	pH 1	(1) ACD
Bioconc. Factor (BCF)	503742	pH 4	(1) ACD
Bioconc. Factor (BCF)	503742	pH 7	(1) ACD
Bioconc. Factor (BCF)	503742	pH 8	(1) ACD
Bioconc. Factor (BCF)	503742	pH 10	(1) ACD
H acceptors (HAC)	0		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	419964	pH 1	(1) ACD
Koc (KOC)	419964	pH 4	(1) ACD
Koc (KOC)	419964	pH 7	(1) ACD
Koc (KOC)	419964	pH 8	(1) ACD
Koc (KOC)	419964	pH 10	(1) ACD
logD (LOGD)	7.81	pH 1	(1) ACD
logD (LOGD)	7.81	pH 4	(1) ACD
logD (LOGD)	7.81	pH 7	(1) ACD
logD (LOGD)	7.81	pH 8	(1) ACD

logD (LOGD)	7.81	pH 10	(1) ACD
logP (LOGP)	7.806+/-0.618		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	452.54		(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software Solaris V4.67 ((C) 1994-2005 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.